Recent developments in organic aerosol modeling

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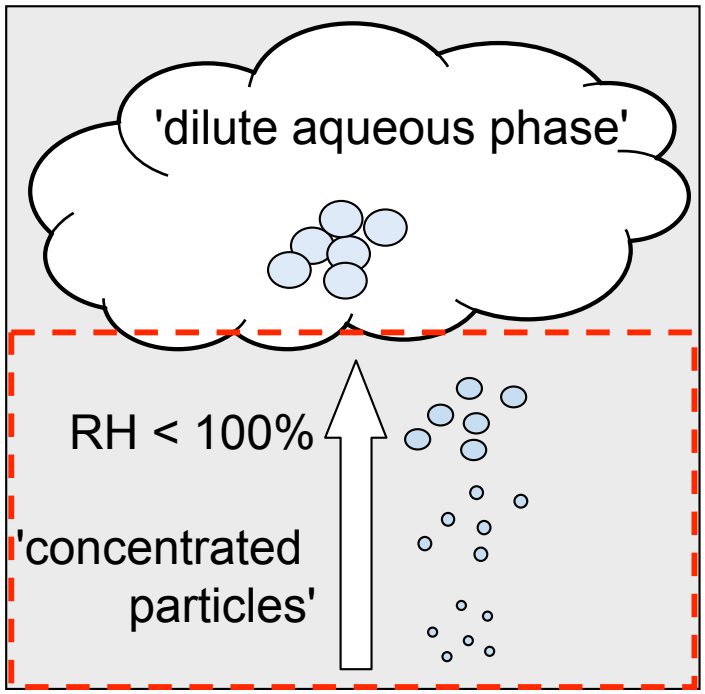
Aerosol processing by aqueous phase chemistry – an important SOA source?



Cloud chemistry

- Oxalate formation

- SOA yields (from isoprene) 0.2 % < Y < 20%

Ervens et al., 2003, 2004, 2008.

Chemical processes in aqueous particles

Several recent lab studies have shown that

(i) products

(ii) rate constants

(iii) reaction mechanisms

are different than in an dilute aqueous phase

Why could chemical processes in haze particle be important?

	Cloud droplets	Aerosols
Life time	minutes	days
LWC	10^{-4} …10^{-3} g/g	10^{-10} …10^{-7} g/g
Solute concentrations	~ μmol L^{-1}	1-10 mol L^{-1}

Reactions such as
Org + *Org* → Org_2 → Org_3 → …
Org + *Sulfate, Ammonium,…* → *Organic -S, -N compounds*
much more likely

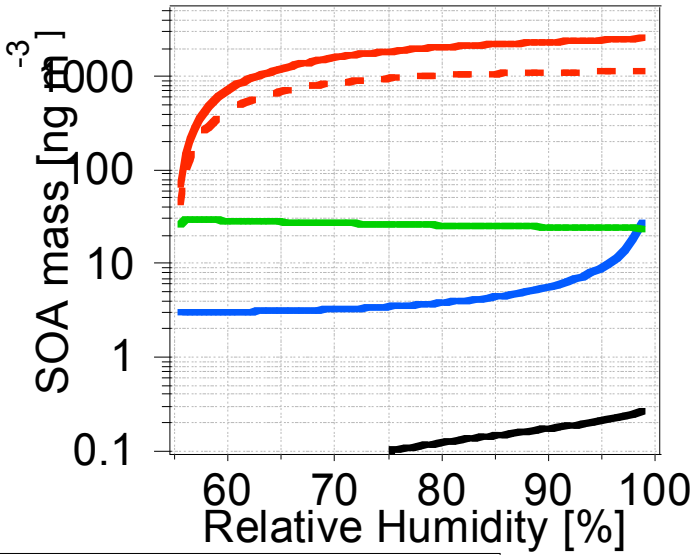
- ***What reaction parameters are known for such processes?***
- And how can they be implemented in models?
- How efficient are these processes in ambient haze particles?

Results using lab data (literature)

Reversible glyoxal uptake

$$K_H^* = K_H \cdot (1 + [Solute] \cdot K_{GlySol})$$

$$Glyoxal + Solute \xleftrightarrow{K(GlySol)} SOA$$

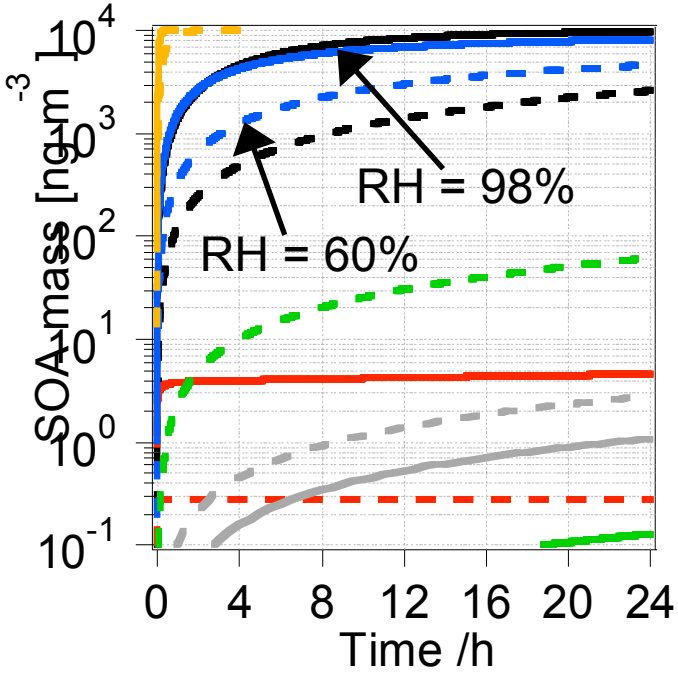


Solute adducts
- in NaCl particles
- in SO_4^{2-} particles
- in fulvic acid particles

Glyoxal self reaction
- Gly --> $(Gly)_2$ --> $(Gly)_3$
- Gly --> $(Gly \cdot H_2O)_2$

Irreversible glyoxal uptake

Gly (+ reactant) ⟶ SOA



- Predicted SOA mass ≤ 10 μg m^{-3} SOA (5 ppb glyoxal)
- Large uncertainties in in suggested reaction parameters

…more details on my poster

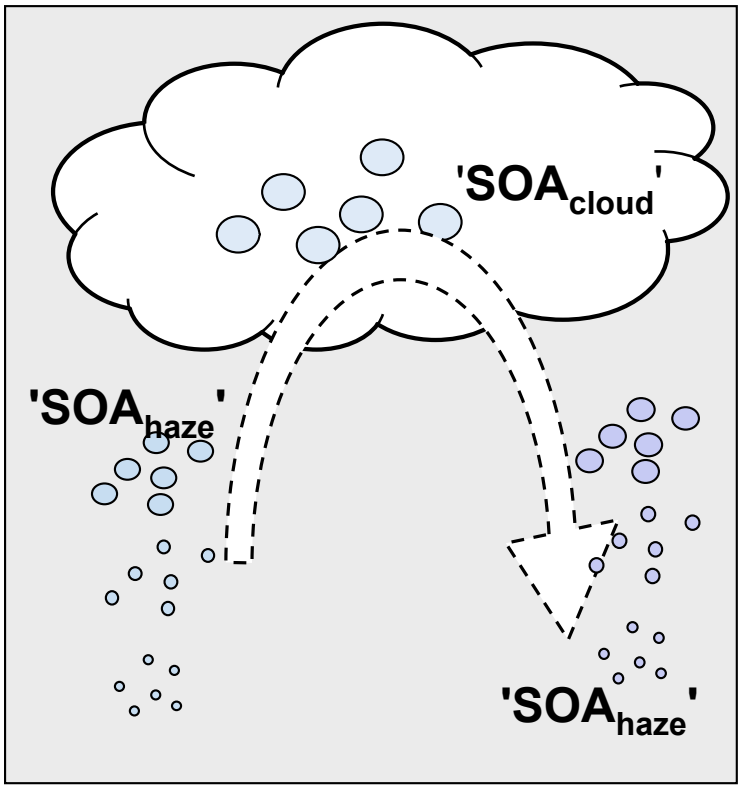
- Gly **bulk rxn**
- Gly **surface rxn**
- Gly + **hν**
- Gly + **NH_4^+**
- Gly + **SO_4^{2-}**
- Gly + **OH** ***'cloud'***

What next?

- Parameterization of 'haze particle SOA formation'

$$m(\text{'SOA haze'}) = f(m_{dry}, \text{composition, RH})$$

- Validation of SOA_{haze} and SOA_{cloud} (= $f(NO_x, LWC, \tau)$) parameterizations



Required input

- VOCs (e.g., glyoxal sources)
- Oxidant levels (O_3, NO_x, …)
- Aerosol parameters (size distribution, composition)
- RH (T, LWC, …) profiles

Questions

- How important is the aqueous phase (haze+cloud) in terms of SOA production
- Can composition/properties of processed aerosol be explained by aqueous chemistry?